

Example 45—Preparation Ethylene/Propylene Copolymer having Isotactic Propylene Segments

The catalyst was prepared by impregnating a toluene solution of 2 μmol rac-[1,2-ethanediylbis(1-indenyl)]zirconium (trans,trans-1,4-diphenylbutadiene) and 6 μmol $\text{B}(\text{C}_6\text{F}_5)_3$ on 0.1 grams of Davison™ 948 silica (available from Davison Chemical Company) which had been treated with 1.0 gram of triethylaluminum/gram of silica. The reactor was charged with 95 psi (650 kPa) of propylene, about 3 psi (20 kPa) of ethylene, 1.5 psi (10 kPa) of hydrogen and 42 psi (290 kPa) of nitrogen. The reactor temperature was set at 70° C. and the catalyst was injected. The temperature remained steady at 70° C. for the duration of the polymerization. 4.6 g of a free-flowing isotactic propylene/ethylene copolymer powder were recovered after 60 minutes. (m pentad=71 percent by ^{13}C NMR analysis).

Example 46—Preparation of rac-1,2-ethanediyl[bis-(1-indenyl)]zirconium(η^4 -1-phenyl-1,3-pentadiene)

In an inert atmosphere glove box 0.896 g (2.14 mmol) of rac-1,2-ethanediyl[bis-(1-indenyl)]zirconium dichloride (in 50 ml of toluene) were combined with 0.309 g of 1-phenyl-1,3-pentadiene (2.14 mmol), followed by addition of 1.8 ml of nBuLi (4.5 mmol, in hexane). The color of the reaction quickly turned red. The reaction mixture was stirred at about 25° C. for 30 minutes followed by heating at reflux for two hours, followed by continued stirring at about 25° C. for 18 hours. The product was collected by filtering, concentrating the filtrate to approximately 30 ml, and cooling the filtrate to approximately -34° C. for about 18 hours. 0.225 g (21.4 Percent) of recrystallized product was isolated as dark red microcrystals after decanting the mother liquor and drying the product under reduced pressure. The product was identified by ^1H NMR spectrum as rac-1,2-ethanediyl[bis-(1-indenyl)]zirconium(η^4 -1-phenyl-1,3-pentadiene).

Example 47—Batch Isotactic Polypropylene Polymerization Using rac-[bis-1,1'-(η^5 -indenyl)-1,2-ethanediyl]zirconium(η^4 -1-phenyl-1,3-pentadiene) and $\text{B}(\text{C}_6\text{F}_5)_3$ with Hydrogen.

The general polymerization procedure was followed using 734 g solvent, 26 Δpsi (180 kPa) hydrogen, 200 g propylene monomer with a reaction temperature of 70° C. and run time of 30 minutes. The catalyst was prepared by combining 4 μmol rac-[bis-1,1'-(η^5 -indenyl)-1,2-ethanediyl]zirconium (η^4 -1-phenyl-1,3-pentadiene) and 4 μmol $\text{B}(\text{C}_6\text{F}_5)_3$ in toluene. 82 g of crystalline polypropylene was obtained.

Example 48—Batch Ethylene/Styrene Polymerization using rac-[1,2-ethanediylbis-(1-indenyl)]zirconium (η^4 -s-trans-1,4-trans,trans-diphenyl-1,3-butadiene) and $\text{B}(\text{C}_6\text{F}_5)_3$ with Hydrogen.

The general polymerization procedure was followed using 365 g solvent, 51 Δpsi (350 kPa) hydrogen, 458 g styrene monomer with a temperature of 70° C. and 200 psig (1.4 MPa) of ethylene on demand and a run time of 15 minutes. The catalyst was prepared by combining 4 μmol of rac-1,2-ethanediyl[bis-(1-indenyl)]zirconium (η^4 -s-trans-1,4-trans,trans-diphenyl-1,3-butadiene) and 4 μmol of

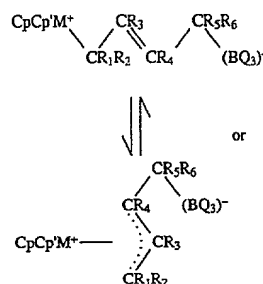
$\text{B}(\text{C}_6\text{F}_5)_3$ in toluene. 19.8 g of an ethylene/styrene copolymer was isolated.

Example 49—Batch Ethylene/1-Octene Polymerization using rac-[1,2-ethanediylbis-(2-methyl-4-phenyl-1-indenyl)]zirconium (η^4 -s-trans-1,4-trans,trans-diphenyl-1,3-butadiene) and $\text{B}(\text{C}_6\text{F}_5)_3$ with Hydrogen.

The general procedure was followed using 741 g solvent, 26 Δpsi (180 kPa) hydrogen, 129 g 1-octene monomer with a temperature of 140° C. and 500 psig (3.4 MPa) of ethylene on demand and run time of 15 minutes. The catalyst was prepared by combining 1 μmol of rac-[1,2-ethanediylbis-(2-methyl-4-phenyl-1-indenyl)]zirconium (η^4 -s-trans-1,4-trans,trans-diphenyl-1,3-butadiene) and 1 μmol $\text{B}(\text{C}_6\text{F}_5)_3$ in toluene. 13.1 g of an ethylene/1-octene copolymer was isolated.

What is claimed is:

1. A metal complex corresponding to one of the two zwitterionic equilibrium structures of the formula:



wherein:

M is titanium, zirconium or hafnium in the +4 formal oxidation state;

Cp and Cp' are each a substituted or unsubstituted cyclopentadienyl group bound in an η^5 bonding mode to M, said substituted cyclopentadienyl group being substituted with from one to five substituents independently selected from the group consisting of hydrocarbyl, silyl, germlyl, halo, cyano, and mixtures thereof, said substituent having up to 20 nonhydrogen atoms, or optionally, two such substituents other than cyano or halo together cause Cp or Cp' to have a fused ring structure, or one substituent on Cp and Cp' forms a linking moiety joining Cp and Cp';

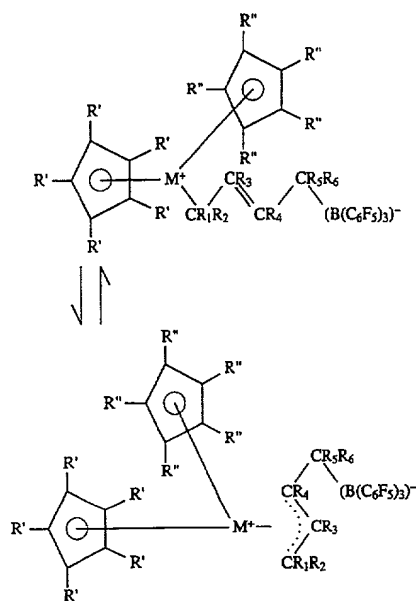
Q independently each occurrence is selected from hydride, dialkylamido, halide, alkoxide, aryloxy, hydrocarbyl, and halosubstituted-hydrocarbyl radicals, said Q having up to 20 carbons with the proviso that in not more than one occurrence is Q halide;

R_1 , R_2 , R_3 , R_4 , R_5 and R_6 are independently hydrogen, hydrocarbyl, silyl and combinations thereof, each of said R_1 to R_6 having up to 20 nonhydrogen atoms; and

B is boron in a valence state of 3.

2. A metal complex according to claim 1 corresponding to the formula:

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wherein:

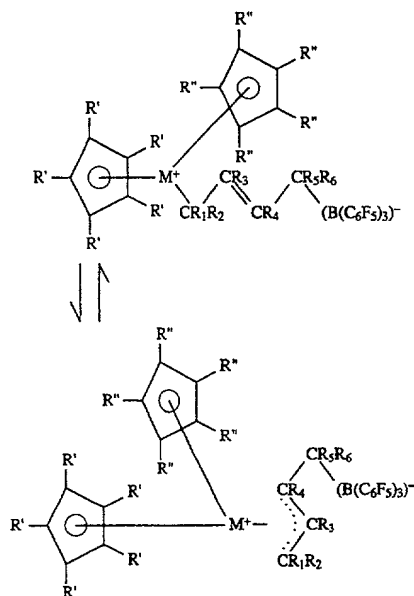
R₁, R₂, R₅ and R₆ are hydrogen;R₃ and R₄ are hydrogen, C₁₋₄ alkyl or phenyl,

M is zirconium in the +4 formal oxidation state, and

R' and R'' in each occurrence are independently selected from the group consisting of hydrogen, hydrocarbyl, silyl, germyl, cyano, halo and combinations thereof, said R' and R'' having up to 20 non-hydrogen atoms each, or adjacent R' groups and/or adjacent R'' groups (when R' and R'' are not hydrogen, halo or cyano) together form a divalent derivative thereby forming a fused ring or one R' and one R'' together (when R' and R'' groups are not hydrogen halo or cyano) combine to form a divalent radical linking the two cyclopentadienyl groups.

3. A metal complex according to claim 1 corresponding to the formula:

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wherein:

M is zirconium in the +4 formal oxidation state;

R₁, R₂, R₅ and R₆ are hydrogenR₃ and R₄ are hydrogen or methyl; and

R' and R'' in each occurrence are independently selected from the group consisting of hydrogen, hydrocarbyl, silyl, germyl, cyano, halo and combinations thereof, said R' and R'' having up to 20 non-hydrogen atoms each, or adjacent R' groups and/or adjacent R'' groups (when R' and R'' are not hydrogen, halo or cyano) together form a divalent derivative thereby forming a fused ring system or one R' and one R'' together (when R' and R'' groups are not hydrogen halo or cyano) combine to form a divalent radical linking the two cyclopentadienyl groups.

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